

Abstract Submitted
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Fullerene Nanobombs for Specific Treatment of Alzheimer Disease (AD): A New Concept in AD Theranostics HEEJAE CHUNG, JOSHUA KIM, ANDREW RHEE, SEONG HYEON LEE, Choice Research Group — When fullerene particle becomes reactive, it easily gives off electrons by the molecular dynamics, and it helps to stabilize the cell affected by Alzheimer Disease caused by the Reactive Oxidative Species (ROS). This project aims to determine the thermodynamic stability of various compounds in Fullerene and its derivatives using a computational quantum physics and chemical physics. Density Functional Theory (DFT) and molecular mechanics are used in order to model the electron properties of the compound. Through the simulation, better and safer functional groups with fullerene, which can be used in the AD treatment with less optimization energy, were found by checking their optimized molecular energy both stereo-chemically and thermo-dynamically. Using the Avogadro and Gamess that allow performing such computations for the compounds, this program shows the optimized geometry energy levels of Fullerene Nano Molecules Used in PDT (Photodynamic Therapy) and fully determines the theoretical values of the structures atomic properties.

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